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13. ABSTRACT (Maximum 200 words)

Calculations were performed on the following problem areas: (1) binding energies and oscillator strengths of excitons in quantum wells in a magnetic field, (2) excitonic luminescence line shape due to interfacial quality in quantum wells in a magnetic field, (3) effect of magnetic field on the excitonic luminescence linewidth in semiconductor alloys, (4) binding energies and oscillator strengths of excitions in quantum wells of different potential profiles in the presence of a magnetic field, and (5) magneto-optics of coupled double quantum wells.

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MAGNETO-OPTICAL PROPERTIES OF QUANTUM WELLS WITH ARBITRARY POTENTIAL PROFILES

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by
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1. Binding Energies and Oscillator Strengths of Excitons In Quantum Wells In A Magnetic Field

We have calculated the binding energies and oscillator strengths of excitons associated with the lowest conduction and valence sub-bands in lattice matched GaAs-$A\ell$GaAs and $In_{0.53}Ga_{0.47}As$ - InP quantum well structures as a function of well size using a variational approach. We assume that the valence sub-bands are decoupled and use the Hamiltonian of an exciton in a magnetic field as given by Greene and Bajaj [1]. We use a trial wave function which consists of a product of the electron and hole sub-band eigenfunctions in a square well multiplied by a function G which describes the internal motion of the exciton. For G we choose a relatively simple form which is known to give good results for the case of zero magnetic field. Using this approach, we calculate the binding energies and oscillator strengths of both the heavy-hole and the light-hole excitons as a function of well size both in the absence and in the presence of an externally applied magnetic field. The magnetic field is assumed to be parallel to the axis of growth [001].

In Fig. 1 we display the variation of the binding energy of the heavy-hole exciton (E_{BH}) as a function of well size in GaAs - $A\ell_{0.3}Ga_{0.7}As$ quantum wells for several values of the magnetic field and in Fig. 2 we show a similar variation for the oscillator strength. We find that for a given well size the values of the binding energies and oscillator strengths of the heavy exciton increase as a function of the magnetic field. The same behavior is also found for the case of the light-hole exciton. We have also done similar calculations in $In_{0.53}Ga_{0.47}As$ - InP quantum well structures and have found essentially the same results. The reason for the enhancement of the values of the binding energies and oscillator strengths is quite simple. The application of the magnetic filed compresses the electron and hole wave function thus increasing their overlap which in turn leads to enhanced values of the binding energies and oscillator strengths.

2. Excitonic Luminescence Line Shape Due to Interfacial Quality in Quantum Wells In A Magnetic Field

We have calculated the luminescence linewidth of both the heavy-hole exciton and the light-hole exciton in lattice matched GaAs - $A\ell$GaAs and $In_{0.53}Ga_{0.47}As$ - InP quantum wells as a function of well size due to interface roughness. Calculations are done both in the absence and in the presence of a magnetic field applied parallel to the axis of growth. The interface is described in terms of microscopic fluctuations δ_1 and δ_2 where δ_1 is the local fluctuation in the well size and δ_2 is the lateral extent of the fluctuation. Using arguments similar to those invoked by Lifshitz [2] to understand the excitation spectra of disordered alloys, we have calculated the probability distribution of fluctuations of the well size over the effective extent of the optical probe, namely, the exciton. Thus this probability distribution is a function of the effective size of the exciton. The line shape is then calculated from this distribution. We have evaluated the full width at half maximum (σ) for both the heavy-hole and the light-hole excitons as a function of the well size and interface parameters δ_1 and δ_2 in the presence of a magnetic field in GaAs - $A\ell_{0.3}Ga_{0.7}As$ and $In_{0.53}Ga_{0.47}As$ - InP quantum well structures.

In Fig. 3 we display the variation of full width at half maximum (σ) of the heavy-hole exciton as a function of well width (L_0) for various values of δ_2 in GaAs - $A\ell_{0.3}Ga_{0.7}As$ quantum wells for a zero value of the magnetic field using $\delta_1 = 2.83$ Å. In Fig. 4 we display the same variation for a magnetic field B = 75 kG. We find that for a given set of values of well width and interface parameters the application of the magnetic field reduces the effective size of the exciton and thus increases the linewidth. The effective size of the exciton in the present work is assumed to be the expectation value of $\pi(x^2 + y^2)$ in the well, namely, the lateral extent of the exciton which is in 'touch' with the interface. This expectation value is calculated using the wave functions described in Section 1. Similar behavior is found for the light-hole exciton in GaAs - $A\ell_{0.3}Ga_{0.7}As$ quantum

wells. Essentially the same results are also found in the case of $In_{0.53}Ga_{.47}As$ - InP quantum well structures. Paper based on this work has been accepted for publication in the Journal of Applied Physics.

3. Effect of Magnetic Field On the Excitonic Luminescence Linewidth In Semiconductor Alloys

We have calculated the excitonic luminescence linewidth in intentionally undoped semiconductor alloys such as AℓGaAs and InGaAs as a function of the applied magnetic field at low temperatures. The dominant mechanism for the excitonic line broadening is due to the statistical potential fluctuations caused by the components of the alloy. In our approach we use the virtual crystal approximation (VCA) to represent the extended electronic states of the alloy and treat the potential fluctuations as perturbation. The probability of a given potential fluctuation in an effective volume of the optical probe, namely, the exciton, is derived using statistical mechanical arguments similar to those used by Lifshitz [2] in his treatment of disordered alloys. We assume that the alloy is completely disordered and there are no clusters present. We further assume that the effective volume of the exciton is given by $\frac{4\pi}{3}\langle r^3\rangle$ where $\langle r^3\rangle$ is the quantum mechanical average of the operator r^3. It was shown by Singh and Bajaj [3] that the values of the linewidths obtained using this effective volume are very close (within 10%) to those obtained using a full quantum mechanical treatment at zero magnetic field. The probability of the potential fluctuations is then related to the linewidth of the excitonic emission as discussed in Ref. [4]. Using this approach we have calculated the linewidth as a function of alloy composition and magnetic field in several semiconductor alloys.

In Fig. 5 we display the variation of the full width at half maximum of the excitonic luminescence transition as a function of the applied magnetic field for various values of the Aℓ concentration (x) for which $A\ell_x Ga_{1-x}As$ has a direct band gap. The lowest band gap of $A\ell_x Ga_{1-x}As$ goes from direct to indirect for value of $x \approx 0.40$. We find that for a given value of the alloy composition x, the excitonic linewidth increases as a function of the magnetic field due to the reduction in the effective volume of the exciton which serves as a probe of the alloy disorder. To calculate the expectation value of r^3 in the presence of a

magnetic field we use the exciton wave functions first employed by Fedders [5]. Similar results are obtained in other semiconductor alloy systems which have direct band gaps. This work is now being prepared for publication.

4. Binding Energies and Oscillator Strengths of Excitons In Quantum Wells of Different Potential Profiles In The Presence of A Magnetic Field

We have calculated the values of the binding energies and oscillator strengths of both the heavy-hole and the light-hole excitons in square, parabolic and asymmetric triangular GaAs - AℓGaAs quantum well structures as a function of the well size in the presence of a magnetic field. We follow a variational approach and assume that the magnetic field is applied along the direction of growth ([001] direction). We consider excitons associated with the lowest conduction and valence sub-bands and neglect the effects of mixing of the valence sub-bands. We first solve for the eigenvalues and eigenfunctions of the particles in the quantum wells using a variational approach. We then average the Coulomb potential along the z direction (directions of growth) using the above mentioned eigenfunctions. We thus obtain a two-dimensional Schrödinger equation for the exciton in the presence of a magnetic field which we solve variationally by expanding the trial wave functions in terms of Gaussian functions in the x and y directions. The exciton binding energies are then obtained by subtracting this value from the sum of the electron and hole sub-band energies in the presence of a magnetic field. The oscillator strengths are calculated by using the well known Fermi's Golden Rule. We do our calculations for both the heavy and the light-hole excitons. A more detailed description of our formalism is given in Ref. [6].

In Fig. 6 we display the band diagram of the asymmetric triangular quantum well consisting of GaAs - $A\ell_{0.3}Ga_{0.7}As$. In Fig. 7 we display the variation of the binding energies of both the heavy-hole and the light-hole excitons as a function of the magnetic field for two different well sizes. In Fig. 8 we display a similar variation for the oscillator strengths. We find that for a given well size the values of the binding energies and oscillator strengths increase as a function of the magnetic field. This is because the application of the magnetic field compresses the excitonic wave function and thus enhances

the values of these quantities. In addition, we find that at zero magnetic field the value of the binding energy of the light-hole exciton is greater than that of the heavy-hole exciton due to the larger reduced mass of the light-hole exciton. As the magnetic field is increased the rate of change of the binding energy of the light-hole exciton is smaller than that of the heavy-hole exciton and for a certain value of the magnetic field the binding energy of the light-hole exciton becomes smaller than that of the heavy-hole exciton. This is due to the fact that it is more difficult to compress the light-hole exciton wave function than the heavy-hole exciton wave function. Similar results are also found in the case of square and parabolic quantum wells. A paper containing a comparative study of the behavior of exctions in square, parabolic and asymmetric triangular quantum wells is now being prepared for publication.

5. Magneto-Optics of Coupled Double Quantum Wells

We have calculated the values of the transition energies, binding energies and oscillator strengths of both the heavy-hole exciton and the light-hole exciton associated with the lowest conduction and valence sub-bands in coupled double GaAs - AℓGaAs square quantum wells as a function of barrier and well thicknesses in the presence of a magnetic field. Again we assume that the magnetic field is applied parallel to the direction of growth.([001]). We follow an approach essentially similar to that outlined in Section 4 and described in much greater detail in Ref.[6]. We assume decoupled valence sub-bands and calculate the sub-band energies of electrons and holes by solving the Schrödinger equation variationally. We enclose this system in a rigid box and expand the trial wave function in a Fourier series of orthonormal functions. In our study we treat the coupled double quantum wells consisting of two GaAs regions of width, W, separated by an AℓGaAs barrier region of width L. These GaAs layers are surrounded by semi-infinite AℓGaAs layers having the same Al concentration as in the barrier region. To approximate the semi-infinite barriers, we take the size of the rigid box to be 2(L+2W). The values of the binding energies and oscillator strengths of the heavy-hole and the light-hole excitons as a function of well and barrier thickness in the presence of magnetic field are then calculated following a procedure similar to that outline in Section 4

In Fig. 9 we display the variation of the binding energy of a heavy-hole exciton as a function of well size W for several different values of the barrier ($A\ell_{0.3}Ga_{0.7}As$) thickness. We find that for a given value of W the binding energy decreases as the barrier thickness is increased. This is because in strongly coupled wells the electron and the hole tunnel readily between the two wells, spending half their time in each. The effective Coulomb interaction obtained by averaging over the electron and the hole motion along the growth direction, is reduced with increasing barrier width by virtue of the fact that an electron and a hole in different wells cannot interact as strongly if the wells are widely separated. For very large

value of L we get a case of an isolated single well with width W. The exciton binding energy in this case is larger than its value for L=0 where the effective size of the well is 2W. For some value of L the exciton binding energy will start increasing till it reaches its maximum value for very large value of L. Our formalism however, is only valid for small values of L.

In Fig. 10 we plot the variation of the binding energy of a heavy-hole exciton as a function of the magnetic field for several values of L for W = 100 Å. In Fig. 11 we plot a similar variation for the oscillator strength. The enhancement of the binding energy and the oscillator strength of the heavy-hole exciton as a function of the magnetic field is again explained in terms of increased overlap between the electron and the hole wave functions. Similar results are obtained for the light-hole exciton. This work is now being prepared for publication.

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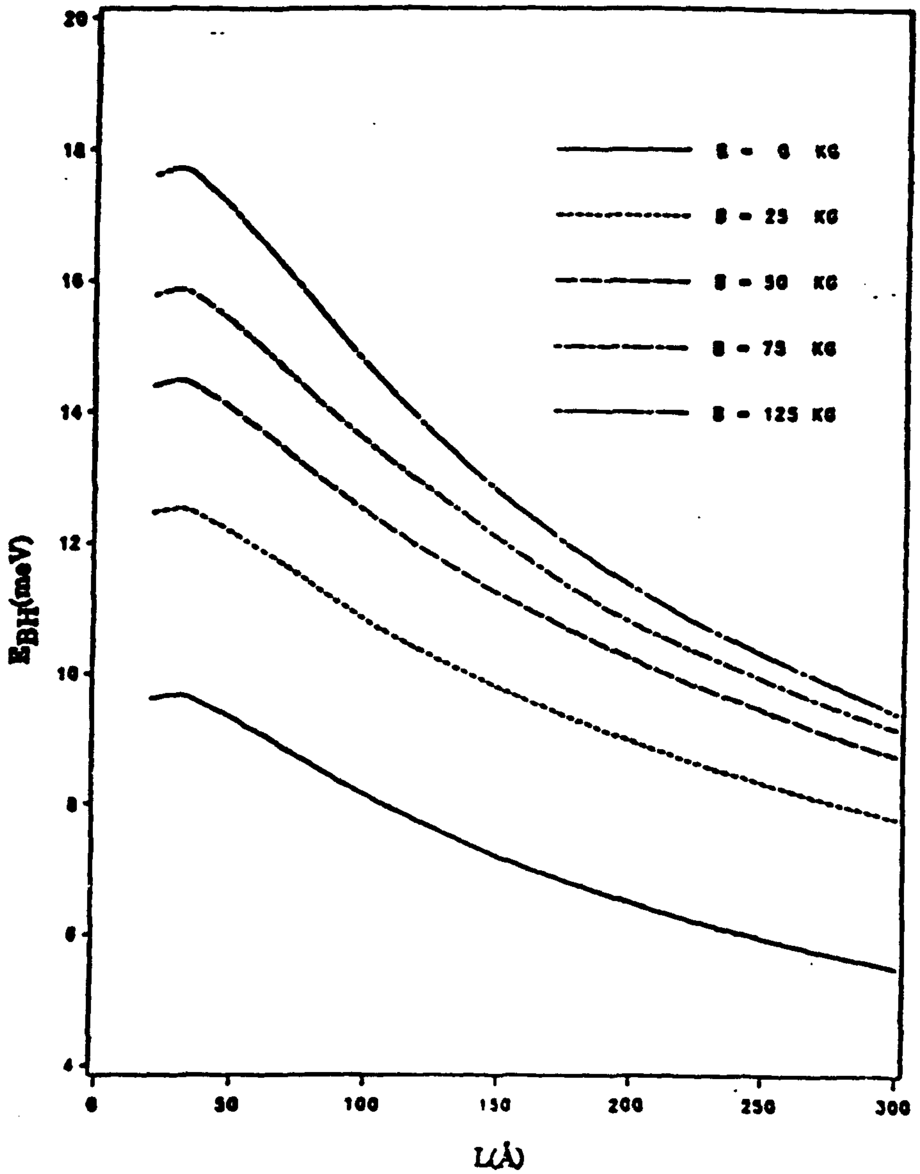

Fig. 1. The variation of the binding energy of the heavy hole exciton(E_{BH}) as a function of well width in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells for several magnetic fields.

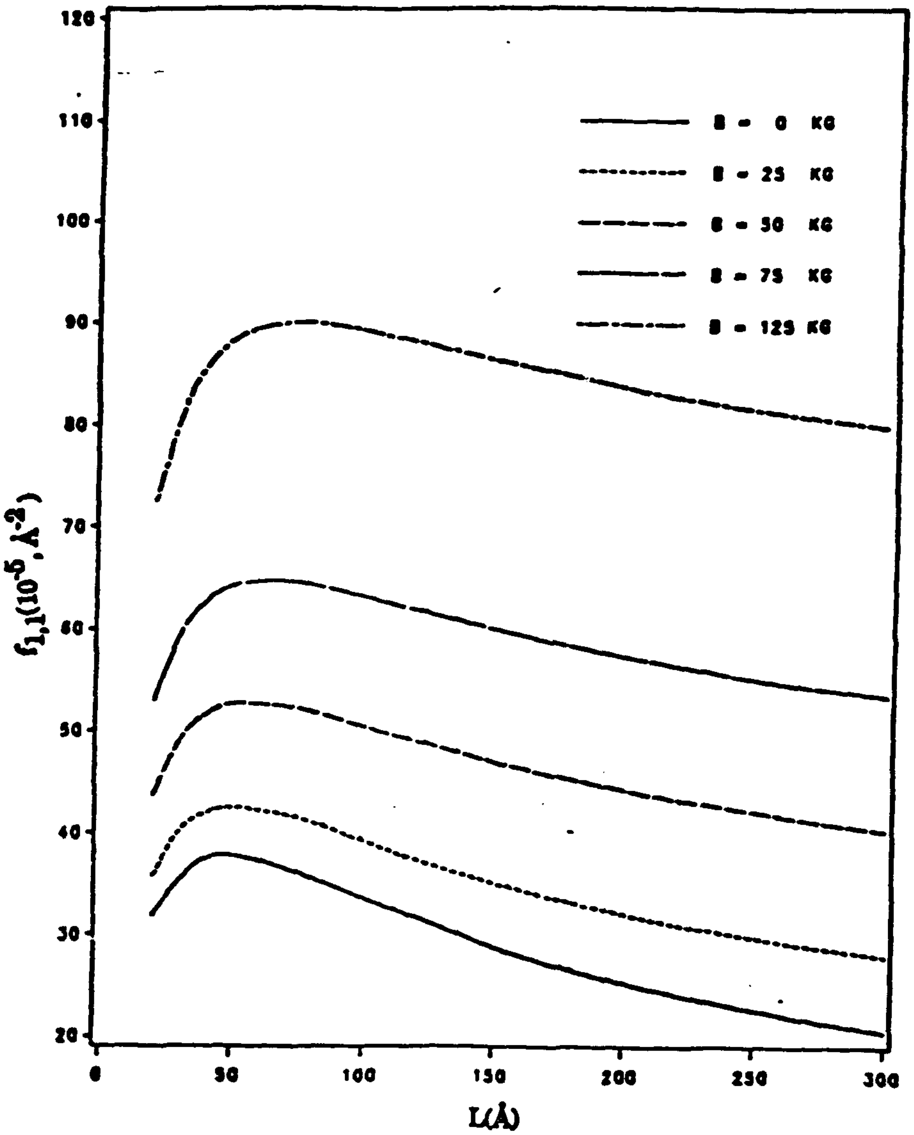

Fig. 2. Oscillator strengths of the heavy hole exciton per unit area vs. well width in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells for several magnetic fields.

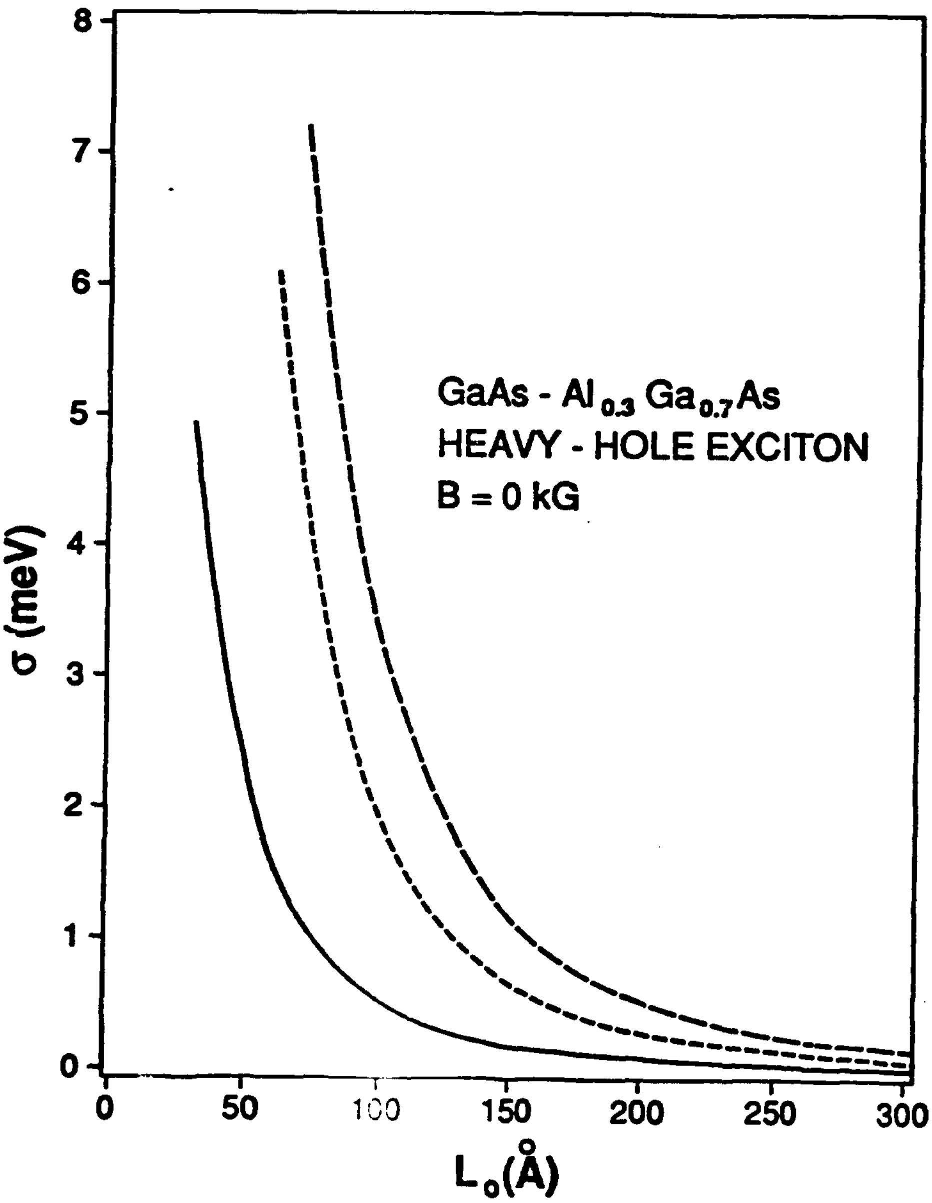

Fig. 3. Variation of full width at half of the heavy-hole exciton as a function of well width for δ2 = 20 Å (solid line) δ2 = 80Å (dotted line) and δ2 = 160Å (dashed line) at B = 0 kG

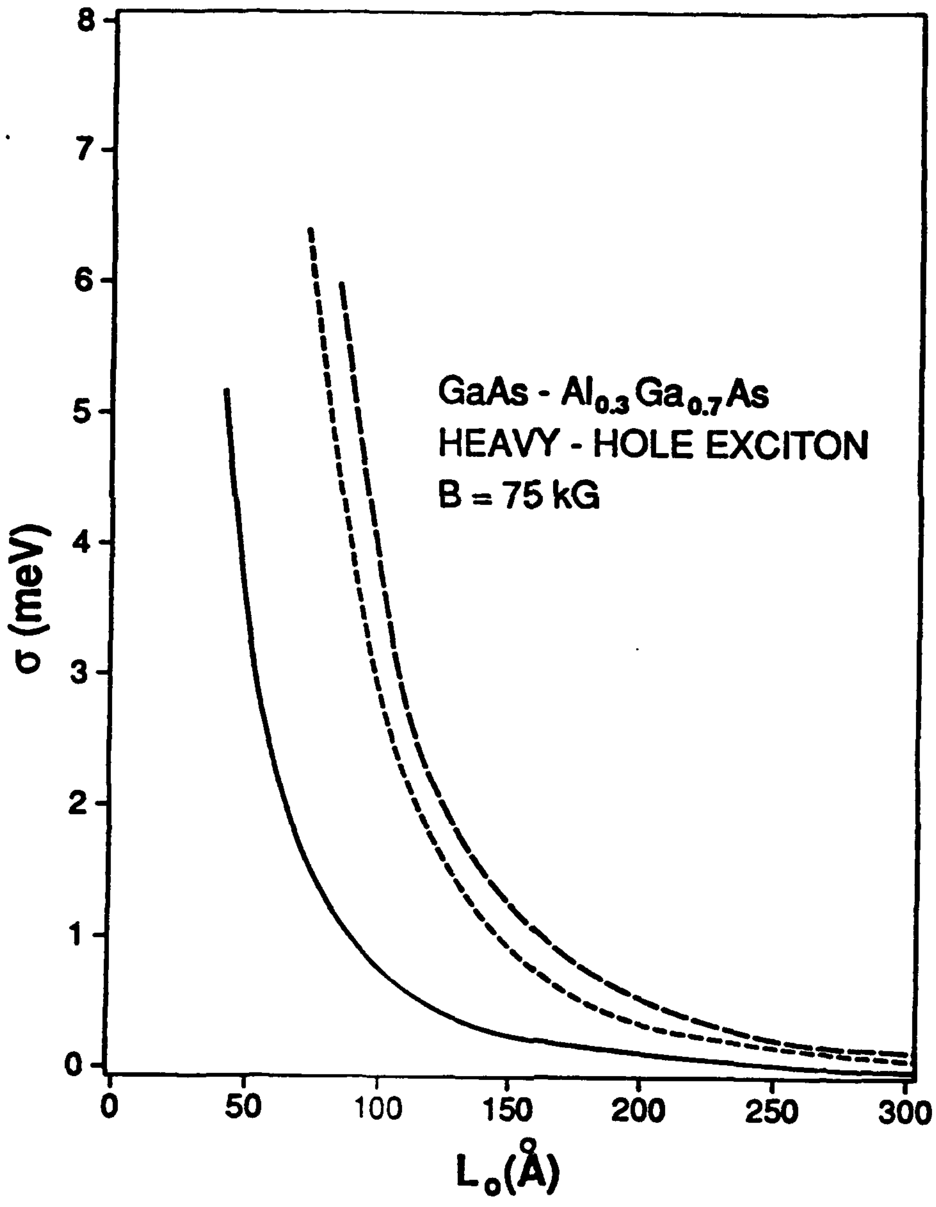

Fig. 4. Variation of full width at half of the heavy-hole exciton as a function of well width for $\delta 2 = 20$ Å (solid line) $\delta 2 = 80$Å (dotted line) and $\delta 2 = 160$Å (dashed line) at B = 75 kG

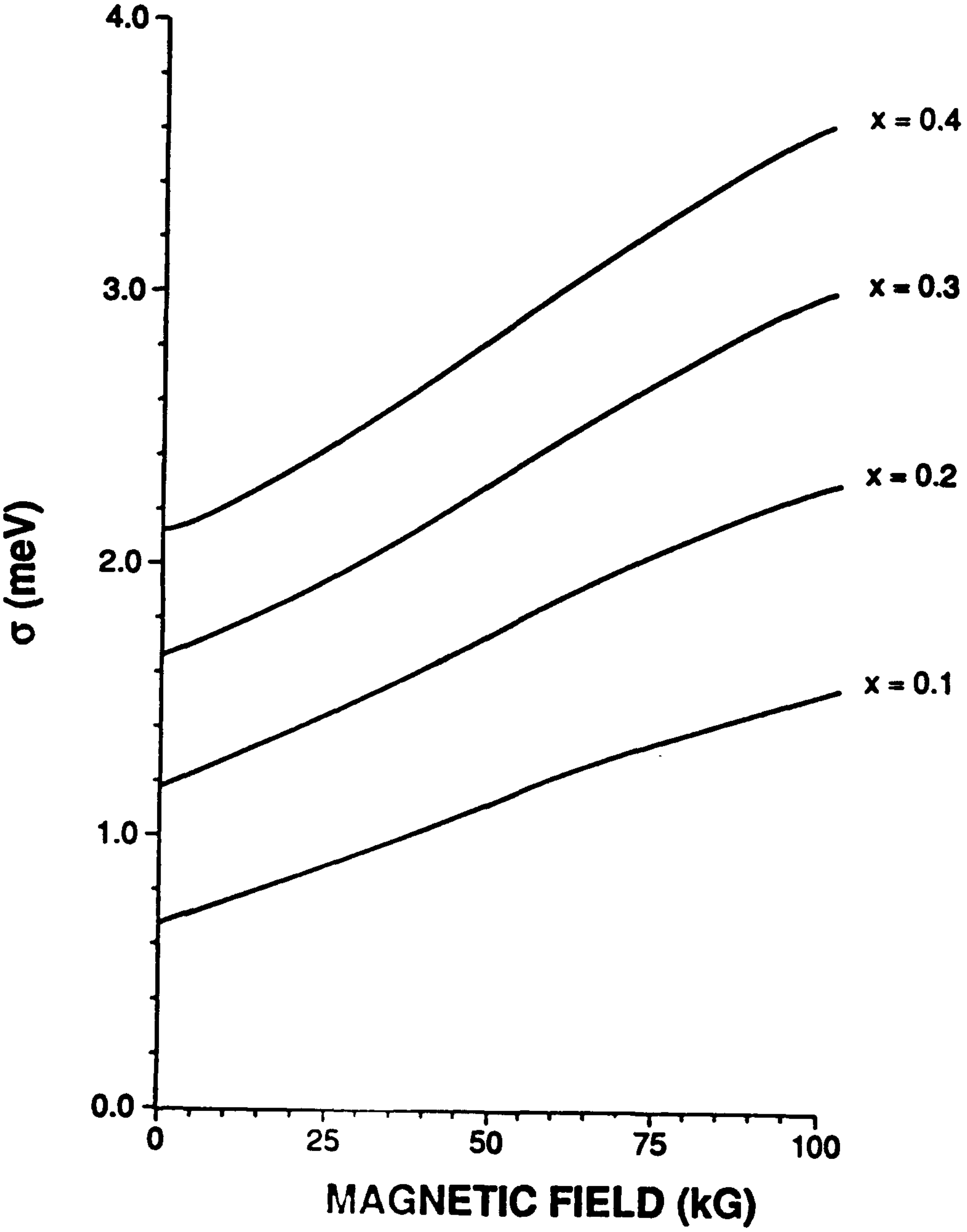

Fig. 5. Variation of full width at half maximum (σ) of the excitonic transition as a function of the magnetic field in $Al_{0.3}Ga_{0.7}As$ for various values of Aℓ concentration x.

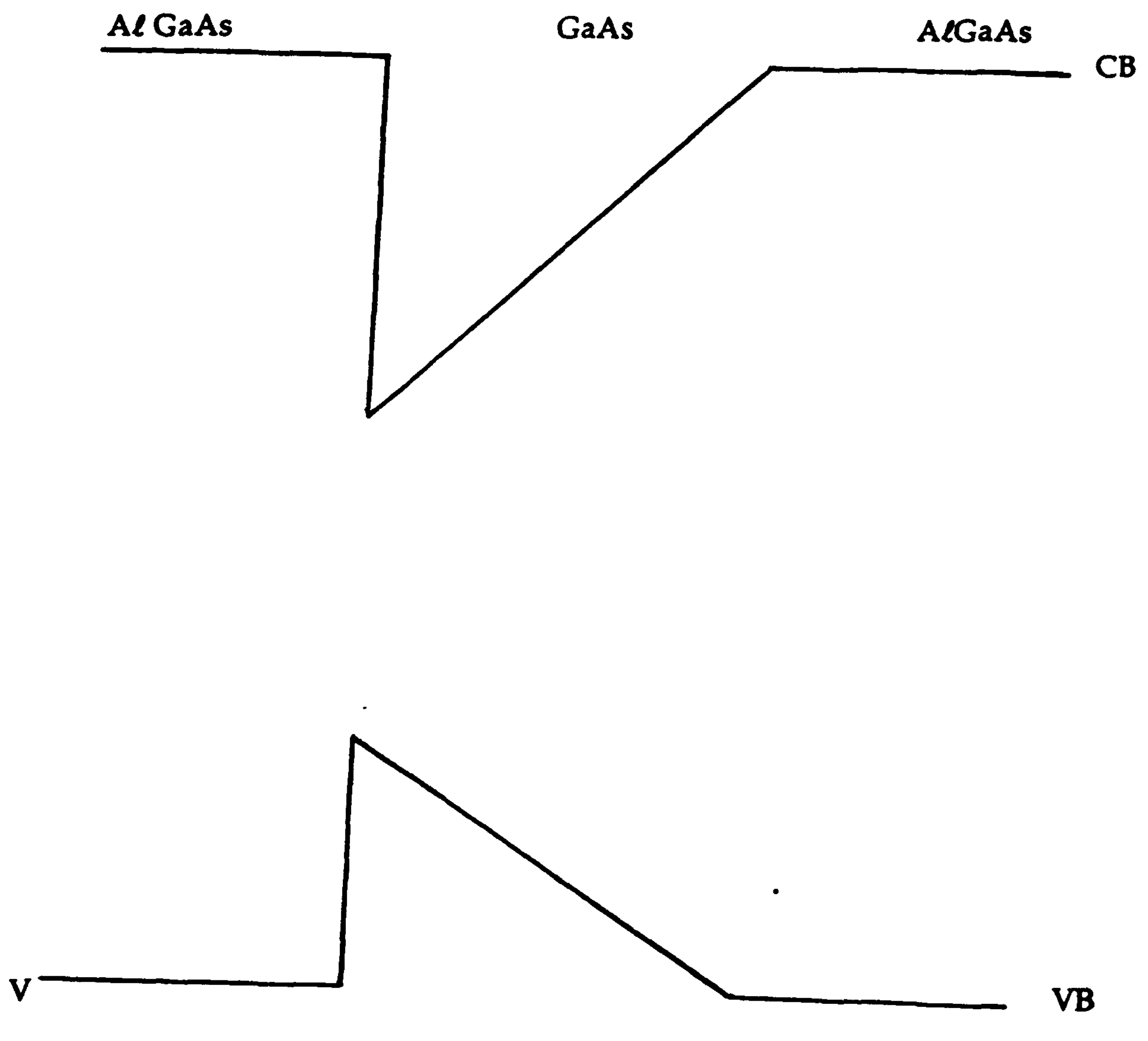

Fig. 6 Schematic band diagram of an asymmetrical triangular quantum well.

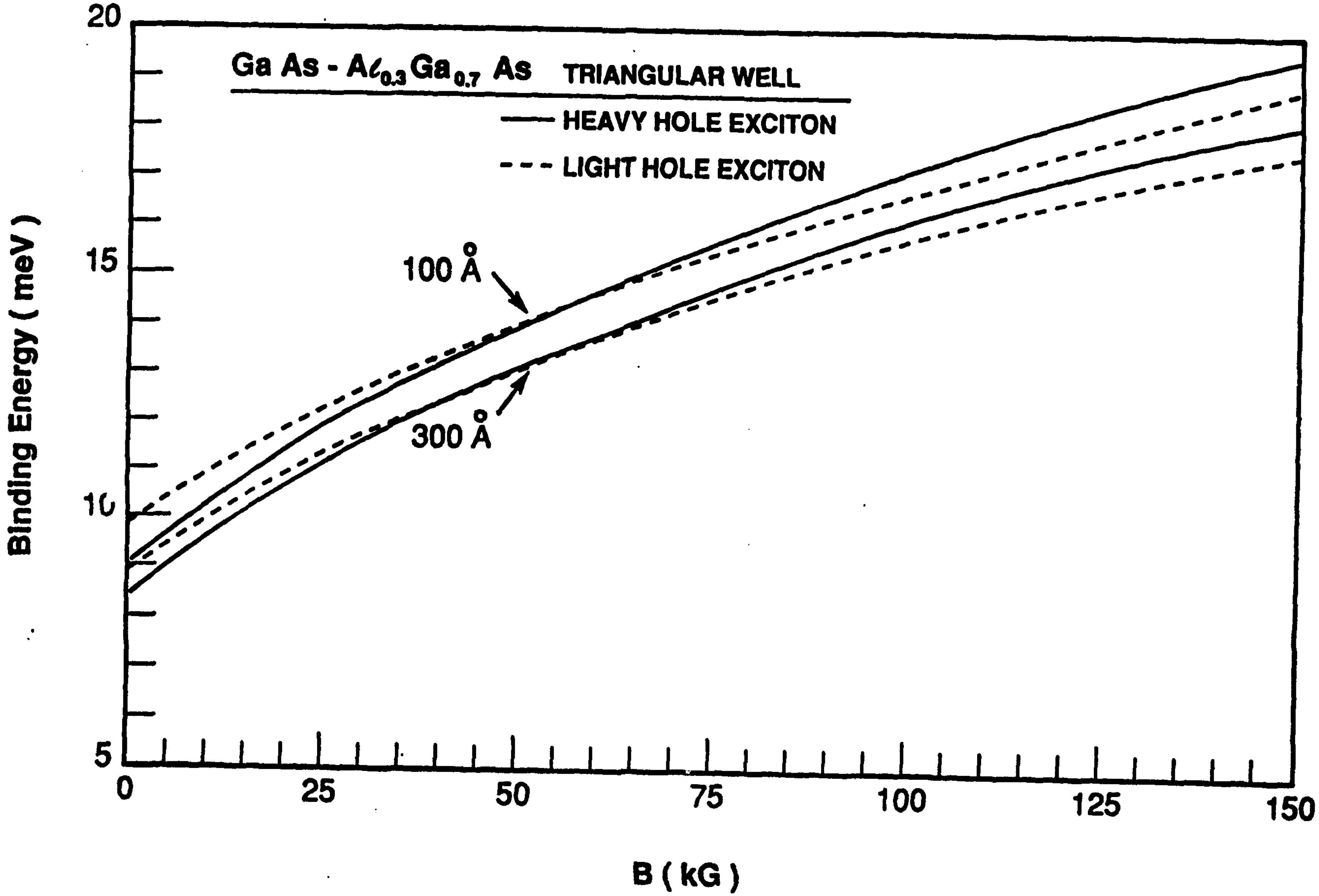

Fig. 7 Variation of the binding energy versus magnetic field for 100 Å and 300 Å wide quantum wells.

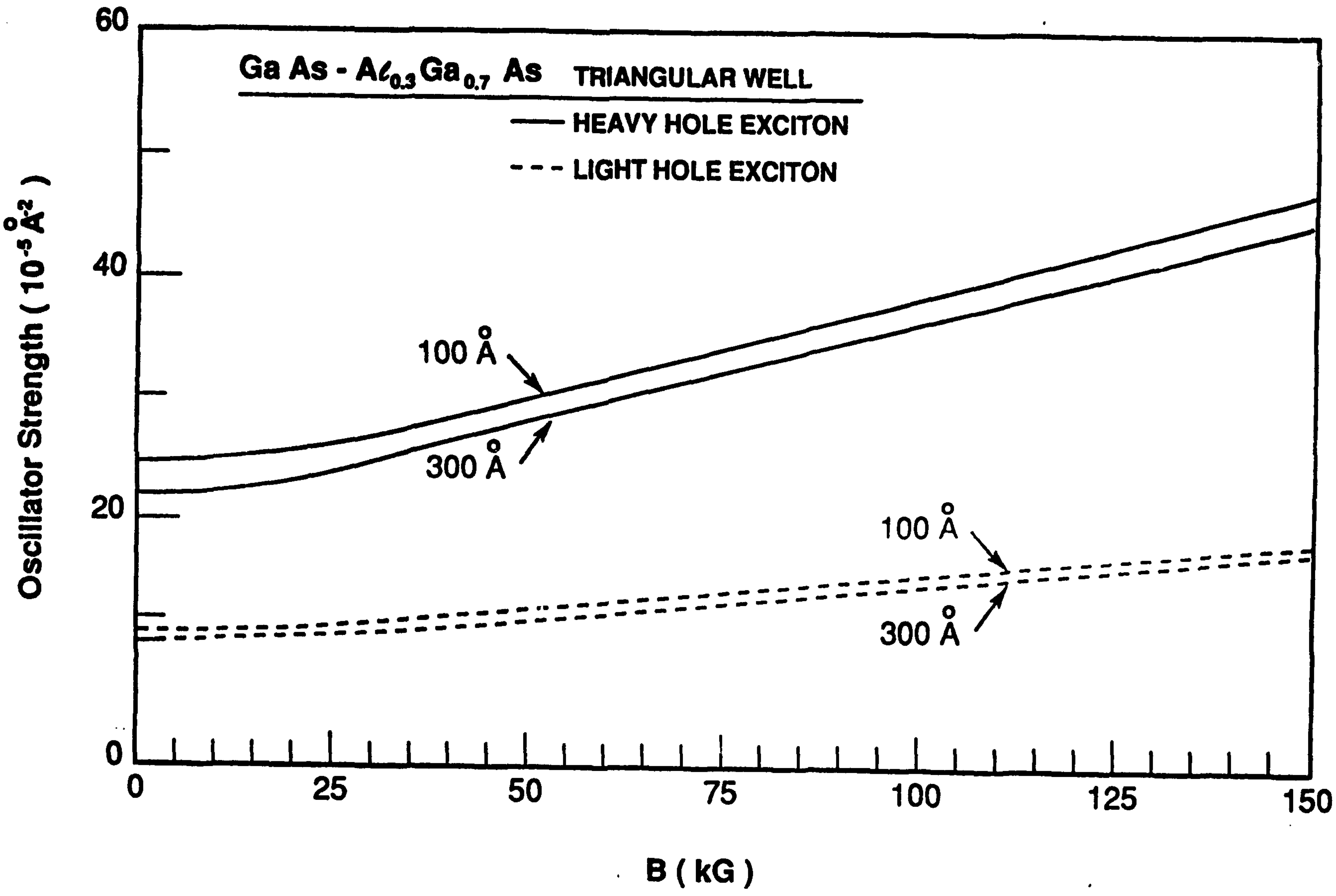

Fig. 8. Variation of the oscillator strength as a function of the magnetic field for 100 Å and 300 Å wide quantum wells.

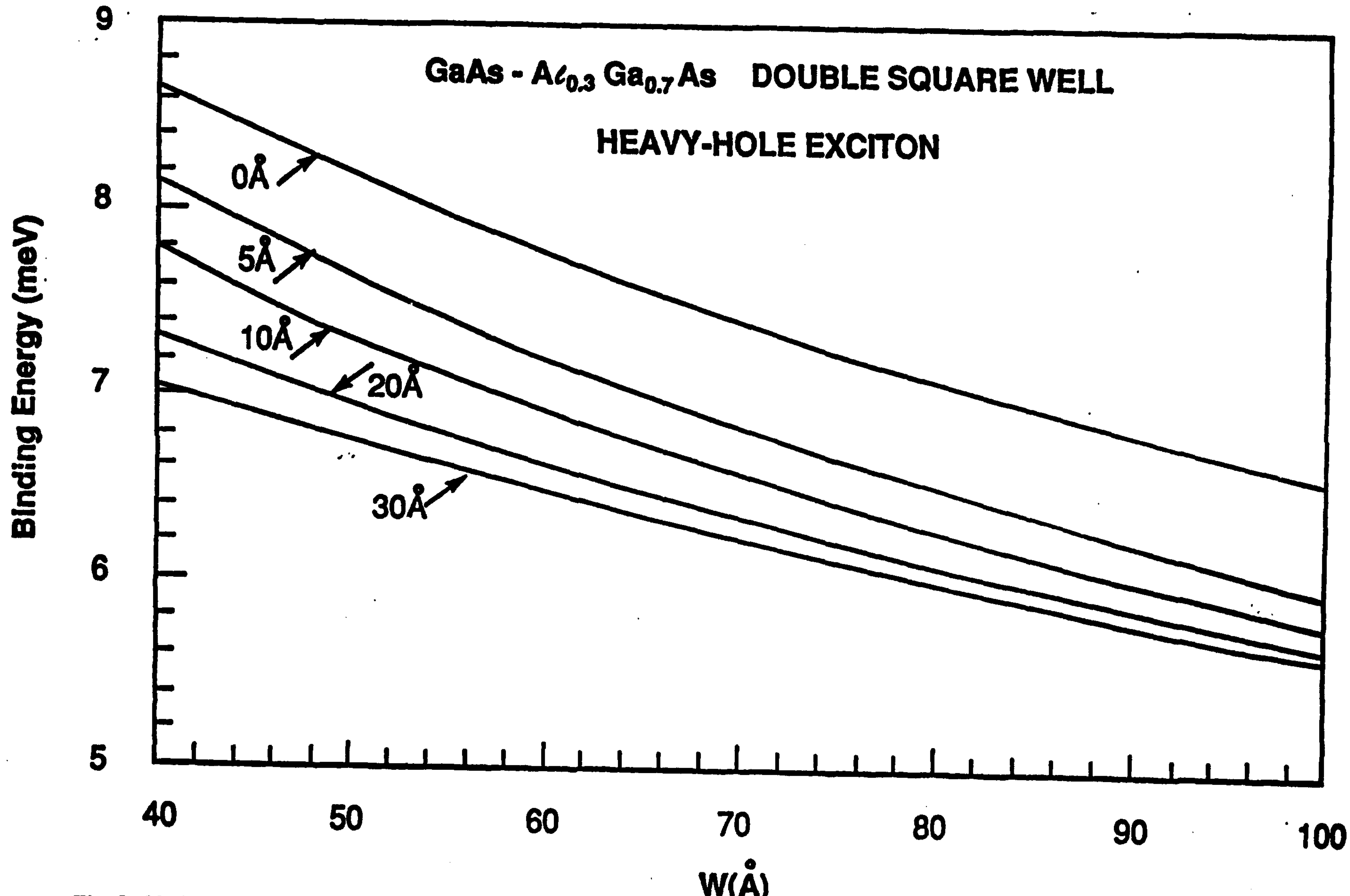

Fig. 9. Variation of the binding energy as a function of well width for various values of the $A\ell_{0.3}Ga_{0.7}As$ barrier widths

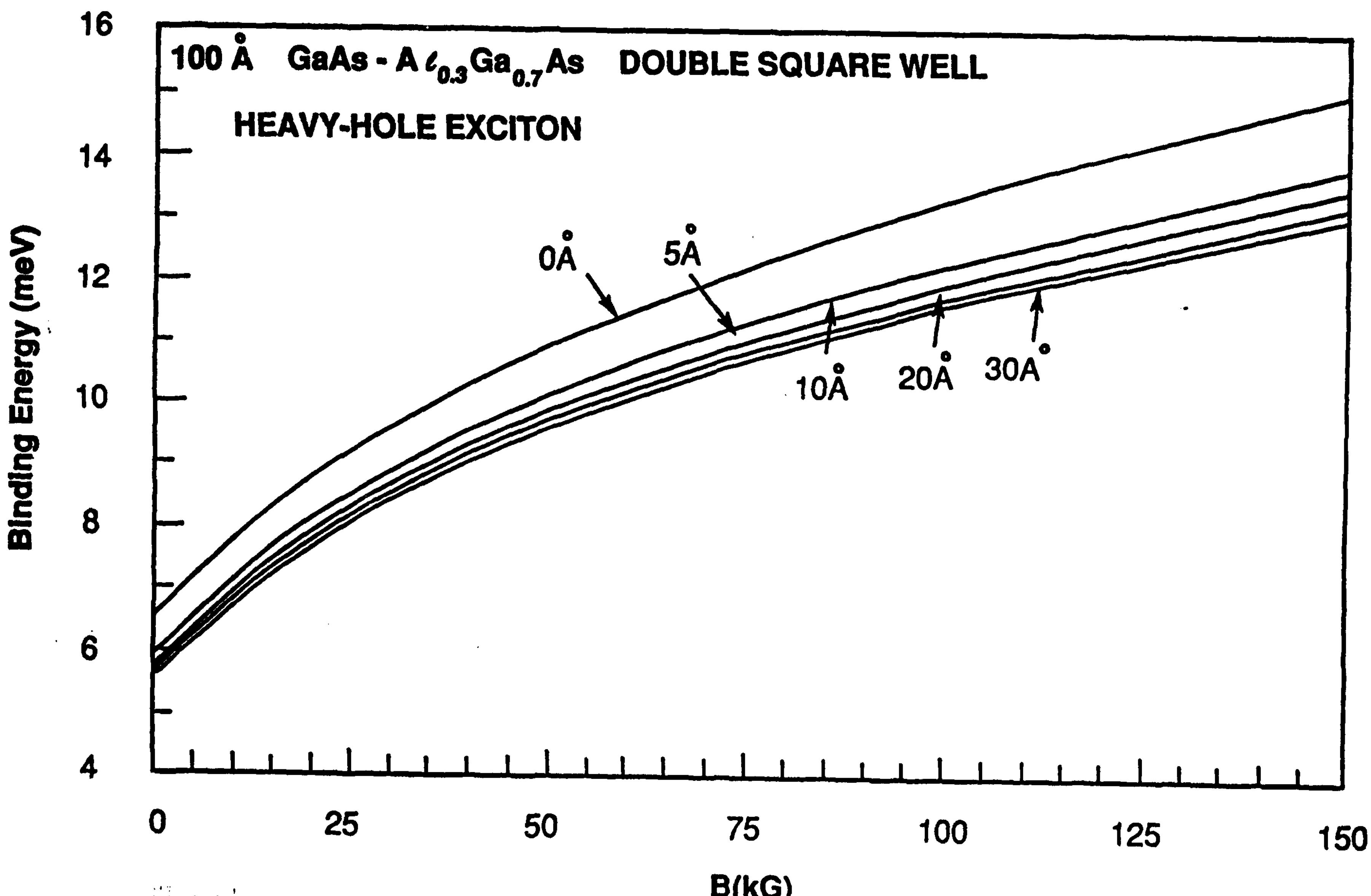

Fig. 10 Binding Energy versus magnetic field for different values of the $Al_{0.3}Ga_{0.7}As$ barrier thickness

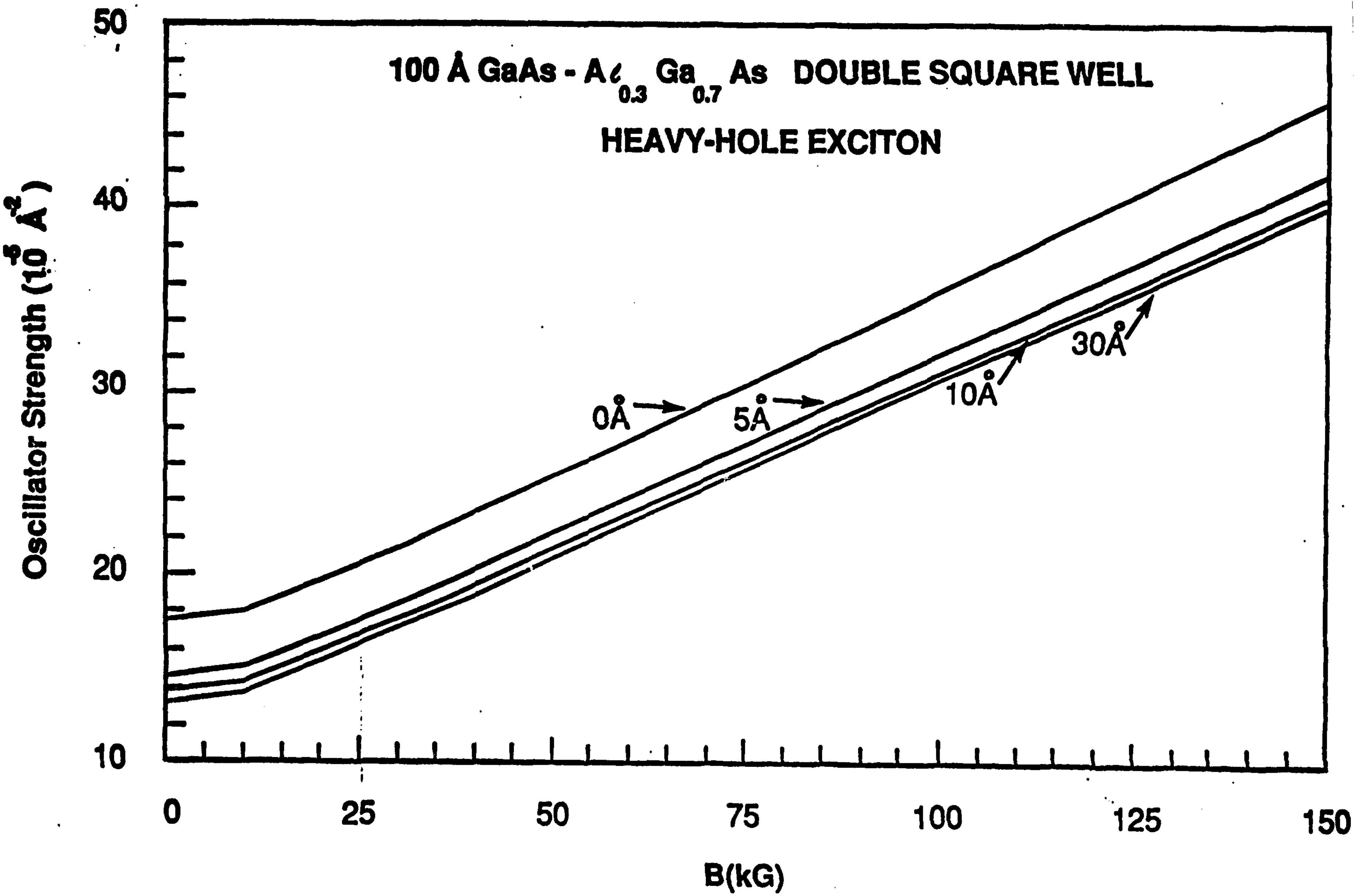

Fig. 11. Oscillator strength versus magnetic field for different values of the $A\ell_{0.3}Ga_{0.7}As$ barrier thickness.